Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 10.3

Global applicability domain: Outside

Local applicability domain index: 7.28e-01

Confidence level: 3.81e-01

Nearest Neighbors from the Training Set

Image not found
1-Octadecanol
Measured: 10.9
Predicted: 10.5

Image not found
1-Hexadecanol
Measured: 9.90
Predicted: 9.79

Image not found
1-Eicosanol
Measured: 12.1
Predicted: 11.2

Image not found
Diphenylamine
Measured: 7.64
Predicted: 8.73

Image not found
Phenacetin
Measured: 9.59
Predicted: 9.23